AUTOFIT: A Program for Fully Automated Fitting of Helmholtz Equations of State

C. Bonsen
Lehrstuhl für Thermodynamik, Ruhr-Universität Bochum, Bochum, Germany

R. Span [C, S]
Thermodynamik und Energietechnik, Universität Paderborn, Paderborn, Germany

W. Wagner
Lehrstuhl für Thermodynamik, Ruhr-Universität Bochum, Bochum, Germany

The numerical stability of accurate empirical equations of state could be significantly improved [1-3] with the introduction of simultaneously optimized functional forms for Helmholtz equations of state. This new approach allows for an accurate description of thermodynamic properties of fluids, for which only limited data sets are available and which could not be described by accurate empirical equations of state before. The feasibility of this concept has been proven for 44 non polar and polar fluids to date. However, to integrate this new type of equations of state into process simulation tools and their fluid-property data-bases, an automated fitting program had to be developed. The "AUTOFIT" program presented in this talk:

reads data from a data base using the PPDX format
develops a consistent data set from the raw data found
fits the 12 coefficients of the equation of state to the selected data
verifies the physical soundness of the fitted equation of state
reports on the quality of the fit.

AUTOFIT has been tested for 30 fluids based on data sets from the DETHERM data base. For 19 fluids, accurate and physically reasonable equations of state could be developed. For 11 fluids, the resulting equations of state showed unreasonable behavior: the available data sets were either too small, too inconsistent, or not well enough distributed. However, physically unreasonable behavior has been automatically detected in all cases. All equations that have passed the integrated tests of AUTOFIT behave physically reasonable. Thus, AUTOFIT is ready to be included into process simulation tools and to make the accuracy of state-of-the-art empirical equations of state available to a multitude of users.

[1] R. Span and W. Wagner: Equations of State for Technical Applications. I. Simultaneously Optimized Functional Forms for Nonpolar and Polar Fluids. International Journal of Thermophysics (2003), in press.
[2] R. Span and W. Wagner: Equations of State for Technical Applications. II. Results for Nonpolar Fluids. International Journal of Thermophysics (2003), in press.
[3] R. Span and W. Wagner: Equations of State for Technical Applications. III. Results for Polar Fluids. International Journal of Thermophysics (2003), in press.